

Benzene, 1,3-dimethyl-2,5-bis-(1-methylethyl)

Inchi:	InChI=1S/C14H22/c1-9(2)13-7-11(5)14(10(3)4)12(6)8-13/h7-10H,1-6H3
InchiKey:	WDFGUVPWPUJTMO-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	Cc1cc(C(C)C)cc(C)c1C(C)C
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	145.64	kJ/mol	Joback Method
hf	-140.73	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.550		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
ripol	1625.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1626.00		NIST Webbook
tb	560.46	K	Joback Method
tc	765.83	K	Joback Method
tf	281.52	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.88	J/mol×K	560.46	Joback Method
cpg	462.03	J/mol×K	594.69	Joback Method
cpg	479.27	J/mol×K	628.92	Joback Method
cpg	495.64	J/mol×K	663.14	Joback Method
cpg	511.14	J/mol×K	697.37	Joback Method

cpg	525.82	J/mol×K	731.60	Joback Method
cpg	539.70	J/mol×K	765.83	Joback Method
dvisc	0.0024229	Pa×s	281.52	Joback Method
dvisc	0.0010915	Pa×s	328.01	Joback Method
dvisc	0.0005993	Pa×s	374.50	Joback Method
dvisc	0.0003757	Pa×s	420.99	Joback Method
dvisc	0.0002584	Pa×s	467.48	Joback Method
dvisc	0.0001902	Pa×s	513.97	Joback Method
dvisc	0.0001473	Pa×s	560.46	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R555987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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